



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 PM GMT

PDB ID : 4KWD  
Title : Crystal structure of Aspergillus terreus aristolochene synthase complexed with (1R,8R,9aS)-1,9a-dimethyl-8-(prop-1-en-2-yl)decahydroquinolizin-5-ium  
Authors : Chen, M.; Al-lami, N.; Janvier, M.; D'Antonio, E.L.; Faraldos, J.A.; Cane, D.E.; Allemann, R.K.; Christianson, D.W.  
Deposited on : 2013-05-23  
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

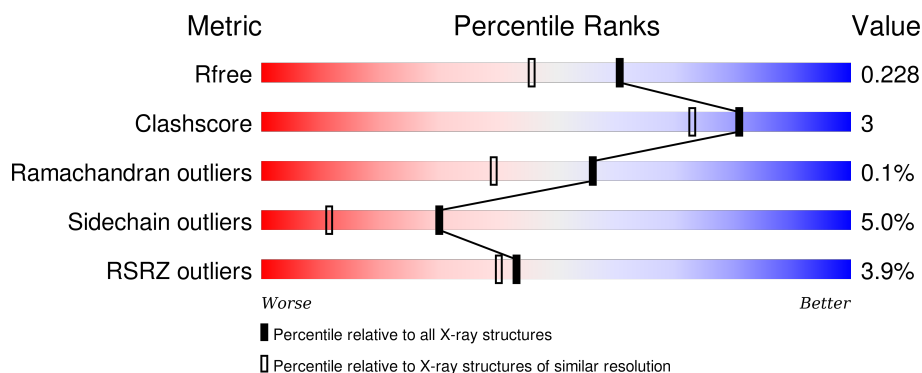
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div>89%</div> <div>8%</div> <div>••</div> </div>
1	B	314	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	C	314	<div> <div>%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
1	D	314	<div> <div>14%</div> <div>80%</div> <div>14%</div> <div>•••</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	JF2	A	405	-	-	-	X
4	JF2	D	405	-	-	-	X
5	GOL	C	406	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aristolochene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	1	0
			2459	1570	415	458	16			
1	B	304	Total	C	N	O	S	0	1	0
			2459	1570	415	458	16			
1	C	304	Total	C	N	O	S	0	1	0
			2459	1570	415	458	16			
1	D	304	Total	C	N	O	S	0	0	0
			2454	1566	415	458	15			

There are 28 discrepancies between the modelled and reference sequences:

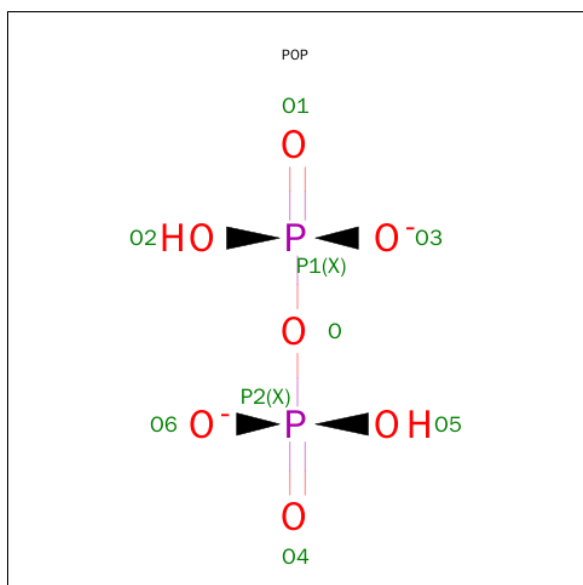
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9UR08
A	2	HIS	-	EXPRESSION TAG	UNP Q9UR08
A	3	HIS	-	EXPRESSION TAG	UNP Q9UR08
A	4	HIS	-	EXPRESSION TAG	UNP Q9UR08
A	5	HIS	-	EXPRESSION TAG	UNP Q9UR08
A	6	HIS	-	EXPRESSION TAG	UNP Q9UR08
A	7	HIS	-	EXPRESSION TAG	UNP Q9UR08
B	1	MET	-	EXPRESSION TAG	UNP Q9UR08
B	2	HIS	-	EXPRESSION TAG	UNP Q9UR08
B	3	HIS	-	EXPRESSION TAG	UNP Q9UR08
B	4	HIS	-	EXPRESSION TAG	UNP Q9UR08
B	5	HIS	-	EXPRESSION TAG	UNP Q9UR08
B	6	HIS	-	EXPRESSION TAG	UNP Q9UR08
B	7	HIS	-	EXPRESSION TAG	UNP Q9UR08
C	1	MET	-	EXPRESSION TAG	UNP Q9UR08
C	2	HIS	-	EXPRESSION TAG	UNP Q9UR08
C	3	HIS	-	EXPRESSION TAG	UNP Q9UR08
C	4	HIS	-	EXPRESSION TAG	UNP Q9UR08
C	5	HIS	-	EXPRESSION TAG	UNP Q9UR08
C	6	HIS	-	EXPRESSION TAG	UNP Q9UR08
C	7	HIS	-	EXPRESSION TAG	UNP Q9UR08

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	EXPRESSION TAG	UNP Q9UR08
D	2	HIS	-	EXPRESSION TAG	UNP Q9UR08
D	3	HIS	-	EXPRESSION TAG	UNP Q9UR08
D	4	HIS	-	EXPRESSION TAG	UNP Q9UR08
D	5	HIS	-	EXPRESSION TAG	UNP Q9UR08
D	6	HIS	-	EXPRESSION TAG	UNP Q9UR08
D	7	HIS	-	EXPRESSION TAG	UNP Q9UR08

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 9 7 2	0	0
2	B	1	Total O P 9 7 2	0	0
2	C	1	Total O P 9 7 2	0	0
2	D	1	Total O P 9 7 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

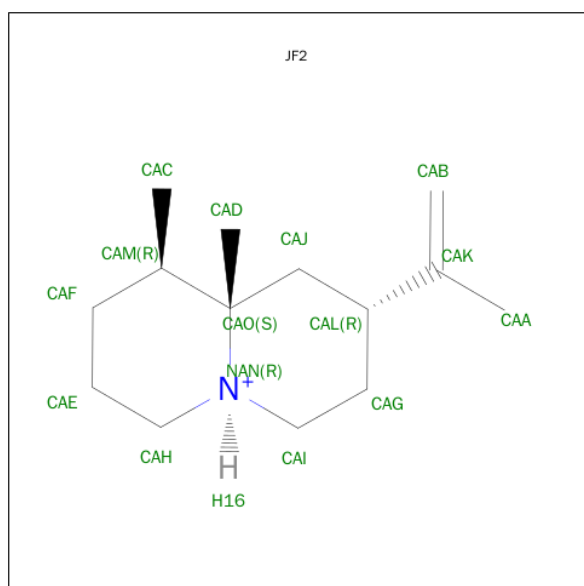
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Mg 3 3	0	0

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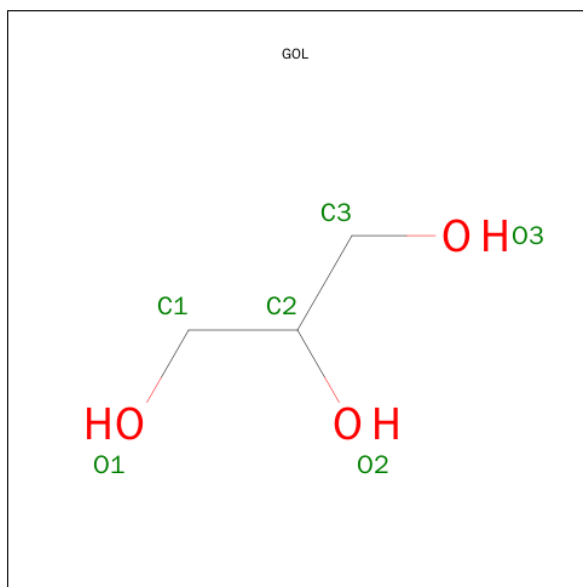
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	D	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		

- Molecule 4 is (1R,5R,8R,9AS)-1,9A-DIMETHYL-8-(PROP-1-EN-2-YL)OCTAHYDRO-2H-QUINOLIZINIUM (three-letter code: JF2) (formula: C<sub>14</sub>H<sub>26</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			15	14	1		
4	B	1	Total	C	N	0	0
			15	14	1		
4	C	1	Total	C	N	0	0
			15	14	1		
4	D	1	Total	C	N	0	0
			15	14	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

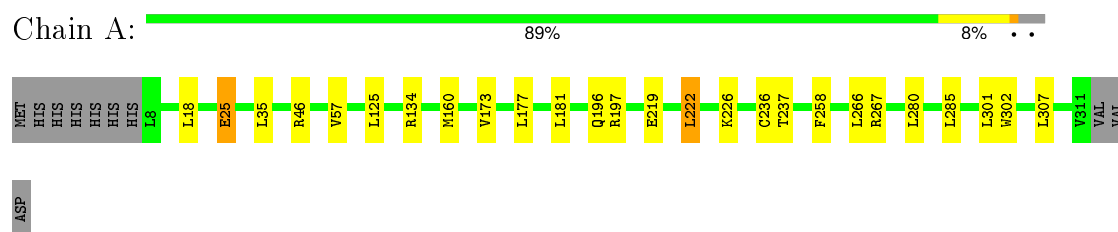
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	336	Total	O	0	0
			336	336		
6	B	353	Total	O	0	0
			353	353		
6	C	229	Total	O	0	0
			229	229		
6	D	131	Total	O	0	0
			131	131		

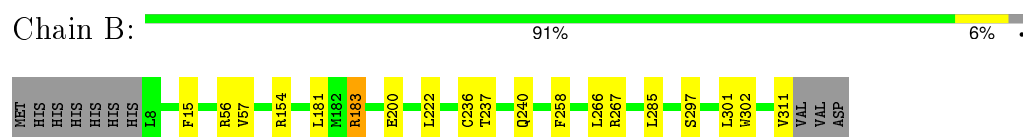
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

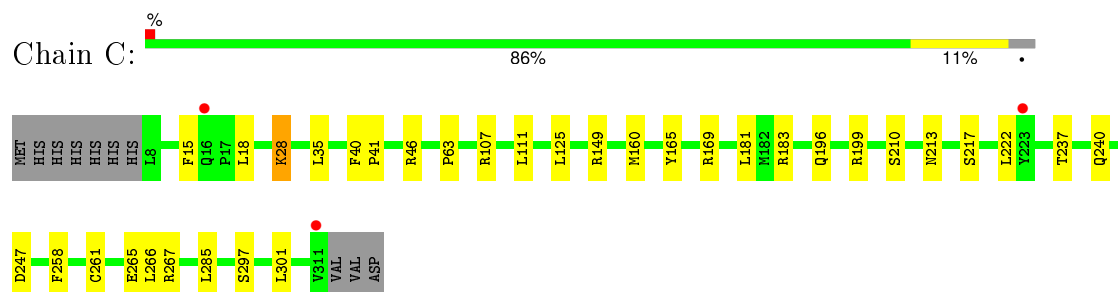
- Molecule 1: Aristolochene synthase



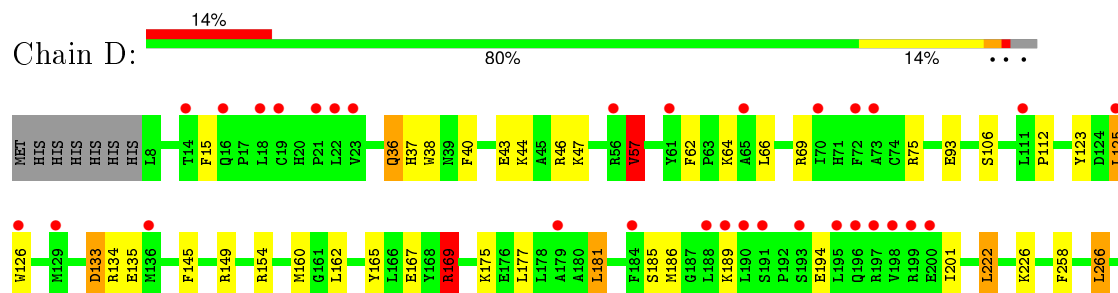
- Molecule 1: Aristolochene synthase



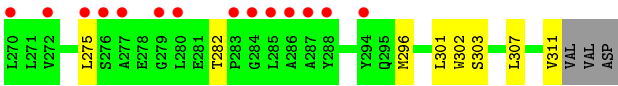
- Molecule 1: Aristolochene synthase



- Molecule 1: Aristolochene synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.86Å 123.86Å 202.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.37 – 1.86 47.37 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.37-1.86) 99.8 (47.37-1.86)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 1.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1370)	Depositor
R, $R_{free}$	0.193 , 0.226 0.197 , 0.228	Depositor DCC
$R_{free}$ test set	7601 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 151240 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, POP, JF2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.78	0/2517	0.80	0/3406
1	B	0.81	0/2517	0.83	3/3406 (0.1%)
1	C	0.68	0/2517	0.74	1/3406 (0.0%)
1	D	0.58	0/2509	0.68	3/3396 (0.1%)
All	All	0.72	0/10060	0.76	7/13614 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	C	107	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	B	183	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	D	169	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	D	57	VAL	CB-CA-C	-6.42	99.20	111.40
1	B	183	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	56	ARG	NE-CZ-NH2	-5.88	117.36	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2459	0	2434	9	0
1	B	2459	0	2434	7	0
1	C	2459	0	2434	13	0
1	D	2454	0	2425	34	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	1	0
2	D	9	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	15	0	26	0	0
4	B	15	0	26	1	0
4	C	15	0	26	1	0
4	D	15	0	26	0	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
6	A	336	0	0	3	0
6	B	353	0	0	5	0
6	C	229	0	0	2	0
6	D	131	0	0	5	0
All	All	11000	0	9847	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:PHE:HE2	1:D:296:MET:HE2	1.50	0.76
1:D:135:GLU:HG2	1:D:189:LYS:HE2	1.72	0.72
1:D:165:TYR:CZ	1:D:169:ARG:HG3	2.31	0.66
1:D:36:GLN:HG2	1:D:37:HIS:CD2	2.31	0.65
4:B:705:JF2:H6	6:B:1153:HOH:O	1.96	0.64
1:D:201:ILE:O	6:D:570:HOH:O	2.14	0.64
1:D:15:PHE:CE2	1:D:296:MET:HE2	2.33	0.64
1:A:197:ARG:HD3	1:A:280:LEU:HB3	1.82	0.62
1:A:35:LEU:O	1:A:46:ARG:NH2	2.32	0.61
1:B:154:ARG:HD2	6:B:949:HOH:O	2.01	0.59
1:C:18:LEU:HD22	1:C:63:PRO:HB2	1.85	0.57
1:B:236:CYS:O	6:B:1126:HOH:O	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LYS:O	1:D:186:MET:HG2	2.06	0.55
1:C:35:LEU:O	1:C:46:ARG:NH2	2.39	0.54
1:A:222:LEU:HD22	1:A:226:LYS:HE3	1.90	0.54
1:D:57:VAL:HG22	1:D:302:TRP:CE2	2.43	0.54
1:D:69:ARG:NH2	1:D:133:ASP:OD1	2.33	0.53
1:D:112:PRO:HD3	1:D:123:TYR:CD1	2.44	0.53
1:D:160:MET:HE1	1:D:165:TYR:HD2	1.74	0.52
1:C:196:GLN:HA	1:C:199:ARG:HD3	1.91	0.52
1:B:183:ARG:NH2	6:B:1116:HOH:O	2.41	0.52
1:B:200:GLU:OE1	1:B:267:ARG:NH2	2.43	0.51
1:C:183:ARG:NH1	6:C:568:HOH:O	2.44	0.51
1:D:57:VAL:HG13	1:D:302:TRP:CG	2.46	0.51
1:A:267:ARG:NH1	6:A:670:HOH:O	2.42	0.50
1:A:25:GLU:HB2	6:A:614:HOH:O	2.11	0.50
1:A:219:GLU:HG2	6:A:653:HOH:O	2.12	0.50
1:D:307:LEU:O	1:D:311:VAL:HG22	2.12	0.49
1:D:75:ARG:HB2	1:D:125:LEU:HD21	1.95	0.48
1:A:160:MET:HE1	1:A:236:CYS:SG	2.54	0.47
1:A:57:VAL:HB	1:A:302:TRP:CE2	2.50	0.47
1:B:15:PHE:HB3	1:B:297:SER:HB3	1.97	0.47
1:D:46:ARG:HD2	6:D:541:HOH:O	2.15	0.46
1:D:66:LEU:HB2	1:D:69:ARG:HD3	1.98	0.46
1:C:213:ASN:O	1:C:217:SER:OG	2.34	0.46
1:D:38:TRP:HB3	1:D:40:PHE:CE1	2.51	0.45
1:D:93:GLU:HG3	1:D:154:ARG:HH22	1.81	0.45
1:D:43:GLU:HG3	1:D:47:LYS:HE2	1.99	0.45
1:D:175:LYS:HG3	6:D:551:HOH:O	2.17	0.45
1:D:15:PHE:HE2	1:D:296:MET:CE	2.27	0.45
1:D:62:PHE:CE1	1:D:181:LEU:HD13	2.52	0.45
1:C:15:PHE:HB3	1:C:297:SER:HB3	1.98	0.45
1:D:222:LEU:HD22	1:D:226:LYS:HE3	2.00	0.44
1:D:266:LEU:HD13	6:D:510:HOH:O	2.17	0.44
1:A:57:VAL:HB	1:A:302:TRP:CD2	2.53	0.43
1:C:149:ARG:NH1	5:C:406:GOL:H11	2.33	0.43
1:C:160:MET:HE1	1:C:165:TYR:HD2	1.83	0.43
1:C:46:ARG:HD2	6:C:619:HOH:O	2.18	0.43
1:C:28:LYS:HA	1:C:28:LYS:HD3	1.81	0.43
1:D:165:TYR:CE2	1:D:169:ARG:HG3	2.53	0.43
1:D:160:MET:HE3	1:D:165:TYR:HB2	2.01	0.43
1:C:169:ARG:HG2	1:C:210:SER:HB3	2.00	0.43
2:C:401:POP:O	4:C:405:JF2:H17	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:CYS:HA	6:B:1023:HOH:O	2.18	0.42
1:C:40:PHE:HA	1:C:41:PRO:HD3	1.76	0.42
1:D:106:SER:HA	1:D:126:TRP:CD1	2.55	0.42
1:B:57:VAL:HB	1:B:302:TRP:CD2	2.54	0.42
1:D:145:PHE:O	1:D:149:ARG:HD2	2.20	0.41
1:C:261:CYS:O	1:C:265:GLU:HG3	2.21	0.41
1:D:57:VAL:HG22	1:D:302:TRP:NE1	2.36	0.41
1:D:296:MET:HB3	1:D:296:MET:HE3	1.69	0.40
1:D:165:TYR:OH	1:D:169:ARG:HD2	2.21	0.40
1:D:303:SER:OG	6:D:555:HOH:O	2.22	0.40
1:D:160:MET:CE	1:D:165:TYR:HD2	2.33	0.40
1:D:194:GLU:OE1	1:D:282:THR:OG1	2.27	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/314 (96%)	300 (99%)	3 (1%)	0	100	100
1	B	303/314 (96%)	300 (99%)	3 (1%)	0	100	100
1	C	303/314 (96%)	299 (99%)	4 (1%)	0	100	100
1	D	302/314 (96%)	293 (97%)	8 (3%)	1 (0%)	46	29
All	All	1211/1256 (96%)	1192 (98%)	18 (2%)	1 (0%)	56	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	133	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/276 (97%)	252 (94%)	15 (6%)	26	9
1	B	267/276 (97%)	258 (97%)	9 (3%)	44	24
1	C	267/276 (97%)	254 (95%)	13 (5%)	31	12
1	D	266/276 (96%)	250 (94%)	16 (6%)	24	7
All	All	1067/1104 (97%)	1014 (95%)	53 (5%)	30	11

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	25	GLU
1	A	125	LEU
1	A	134	ARG
1	A	173	VAL
1	A	177	LEU
1	A	181	LEU
1	A	196	GLN
1	A	222	LEU
1	A	237	THR
1	A	258	PHE
1	A	266	LEU
1	A	285	LEU
1	A	301	LEU
1	A	307	LEU
1	B	181	LEU
1	B	222	LEU
1	B	237	THR
1	B	240	GLN
1	B	258	PHE
1	B	266	LEU
1	B	285	LEU
1	B	301	LEU
1	B	311	VAL

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Mol	Chain	Res	Type
1	C	28	LYS
1	C	111	LEU
1	C	125	LEU
1	C	181	LEU
1	C	222	LEU
1	C	237	THR
1	C	240	GLN
1	C	247	ASP
1	C	258	PHE
1	C	266	LEU
1	C	267	ARG
1	C	285	LEU
1	C	301	LEU
1	D	36	GLN
1	D	44	LYS
1	D	57	VAL
1	D	125	LEU
1	D	134	ARG
1	D	162	LEU
1	D	167	GLU
1	D	169	ARG
1	D	177	LEU
1	D	181	LEU
1	D	185	SER
1	D	222	LEU
1	D	258	PHE
1	D	266	LEU
1	D	275	LEU
1	D	301	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	196	GLN
1	C	39	ASN
1	D	132	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	POP	A	401	3	8,8,8	0.82	0	13,13,13	1.08	1 (7%)
4	JF2	A	405	-	14,16,16	0.89	1 (7%)	17,24,24	2.09	5 (29%)
2	POP	B	704	3	8,8,8	0.84	0	13,13,13	1.22	1 (7%)
4	JF2	B	705	-	14,16,16	0.62	0	17,24,24	2.19	5 (29%)
5	GOL	B	706	-	5,5,5	0.20	0	5,5,5	0.72	0
2	POP	C	401	3	8,8,8	0.88	0	13,13,13	1.41	2 (15%)
4	JF2	C	405	-	14,16,16	0.79	1 (7%)	17,24,24	1.53	4 (23%)
5	GOL	C	406	-	5,5,5	0.19	0	5,5,5	0.67	0
2	POP	D	401	3	8,8,8	1.08	0	13,13,13	1.17	1 (7%)
4	JF2	D	405	-	14,16,16	0.74	1 (7%)	17,24,24	1.31	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POP	A	401	3	-	0/6/6/6	0/0/0/0
4	JF2	A	405	-	-	0/4/32/32	0/2/2/2
2	POP	B	704	3	-	0/6/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	JF2	B	705	-	-	0/4/32/32	0/2/2/2
5	GOL	B	706	-	-	0/4/4/4	0/0/0/0
2	POP	C	401	3	-	0/6/6/6	0/0/0/0
4	JF2	C	405	-	-	0/4/32/32	0/2/2/2
5	GOL	C	406	-	-	0/4/4/4	0/0/0/0
2	POP	D	401	3	-	0/6/6/6	0/0/0/0
4	JF2	D	405	-	-	0/4/32/32	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	405	JF2	CAO-CAM	-2.23	1.52	1.55
4	C	405	JF2	CAO-CAM	-2.12	1.52	1.55
4	A	405	JF2	CAH-NAN	2.33	1.50	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	705	JF2	CAI-NAN-CAH	-5.49	104.67	110.55
2	C	401	POP	P2-O-P1	-4.17	121.02	132.73
4	A	405	JF2	CAE-CAF-CAM	-3.93	106.11	112.66
2	B	704	POP	P2-O-P1	-3.80	122.06	132.73
4	B	705	JF2	CAD-CAO-CAJ	-3.58	105.15	110.74
2	A	401	POP	P2-O-P1	-3.39	123.21	132.73
4	A	405	JF2	CAO-CAJ-CAL	-3.03	108.43	114.44
4	C	405	JF2	CAD-CAO-CAM	-2.95	107.34	112.04
4	A	405	JF2	CAJ-CAL-CAK	-2.82	108.06	112.42
4	D	405	JF2	CAI-NAN-CAH	-2.77	107.58	110.55
4	B	705	JF2	CAO-CAJ-CAL	-2.71	109.07	114.44
4	C	405	JF2	CAO-CAJ-CAL	-2.69	109.11	114.44
4	B	705	JF2	CAJ-CAL-CAG	-2.68	106.57	109.70
4	A	405	JF2	CAI-NAN-CAH	-2.58	107.79	110.55
4	C	405	JF2	CAI-NAN-CAH	-2.55	107.82	110.55
4	B	705	JF2	CAG-CAL-CAK	-2.41	106.99	113.15
4	C	405	JF2	CAE-CAF-CAM	-2.31	108.81	112.66
2	C	401	POP	O-P2-O4	-2.16	100.94	107.70
2	D	401	POP	O5-P2-O6	2.29	119.85	110.61
4	A	405	JF2	CAF-CAE-CAH	4.19	116.57	110.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	705	JF2	1	0
2	C	401	POP	1	0
4	C	405	JF2	1	0
5	C	406	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	304/314 (96%)	-0.56	0 100 100	10, 17, 32, 50	0
1	B	304/314 (96%)	-0.56	0 100 100	10, 15, 27, 41	0
1	C	304/314 (96%)	-0.27	3 (0%) 84 84	13, 25, 44, 58	0
1	D	304/314 (96%)	0.71	45 (14%) 3 3	21, 38, 66, 96	0
All	All	1216/1256 (96%)	-0.17	48 (3%) 43 40	10, 23, 49, 96	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	LEU	6.0
1	D	277	ALA	5.0
1	D	195	LEU	4.7
1	D	279	GLY	4.4
1	D	18	LEU	3.7
1	D	275	LEU	3.7
1	D	188	LEU	3.6
1	D	126	TRP	3.5
1	D	19	CYS	3.4
1	D	72	PHE	3.3
1	D	285	LEU	3.2
1	D	287	ALA	3.2
1	D	197	ARG	3.1
1	D	70	ILE	2.9
1	D	193	SER	2.9
1	D	272	VAL	2.9
1	D	196	GLN	2.9
1	D	23	VAL	2.8
1	D	191	SER	2.7
1	D	190	LEU	2.7
1	C	311	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	61	TYR	2.6
1	D	199	ARG	2.6
1	D	65	ALA	2.6
1	D	22	LEU	2.5
1	D	184	PHE	2.5
1	D	129	MET	2.4
1	D	136	MET	2.4
1	D	56	ARG	2.4
1	D	286	ALA	2.4
1	D	270	LEU	2.3
1	D	111	LEU	2.3
1	D	189	LYS	2.2
1	C	16	GLN	2.2
1	D	288	TYR	2.2
1	D	125	LEU	2.2
1	D	14	THR	2.2
1	D	284	GLY	2.2
1	D	16	GLN	2.2
1	D	200	GLU	2.2
1	D	283	PRO	2.1
1	D	21	PRO	2.1
1	D	294	TYR	2.1
1	D	179	ALA	2.1
1	D	276	SER	2.1
1	D	73	ALA	2.0
1	C	223	TYR	2.0
1	D	198	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	C	406	6/6	0.88	0.24	4.69	24,40,46,49	0
4	JF2	A	405	15/15	0.91	0.12	2.81	18,21,26,28	0
4	JF2	D	405	15/15	0.85	0.19	2.56	36,45,53,54	0
4	JF2	C	405	15/15	0.94	0.11	1.99	25,31,35,37	0
3	MG	B	702	1/1	1.00	0.10	1.40	10,10,10,10	0
4	JF2	B	705	15/15	0.93	0.11	1.38	18,22,25,27	0
2	POP	D	401	9/9	0.95	0.11	0.48	23,28,28,29	0
3	MG	A	403	1/1	0.98	0.07	0.21	13,13,13,13	0
2	POP	B	704	9/9	0.99	0.09	0.21	8,10,10,13	0
2	POP	A	401	9/9	0.99	0.08	0.20	10,11,12,13	0
3	MG	D	403	1/1	0.93	0.08	-0.60	24,24,24,24	0
5	GOL	B	706	6/6	0.97	0.07	-0.76	25,26,29,33	0
2	POP	C	401	9/9	0.98	0.07	-1.36	18,19,22,24	0
3	MG	C	402	1/1	0.98	0.05	-3.06	19,19,19,19	0
3	MG	B	701	1/1	1.00	0.10	-	12,12,12,12	0
3	MG	C	404	1/1	0.96	0.07	-	22,22,22,22	0
3	MG	D	402	1/1	0.96	0.06	-	23,23,23,23	0
3	MG	D	404	1/1	0.88	0.11	-	24,24,24,24	0
3	MG	A	402	1/1	0.98	0.06	-	14,14,14,14	0
3	MG	B	703	1/1	1.00	0.08	-	10,10,10,10	0
3	MG	A	404	1/1	0.99	0.05	-	11,11,11,11	0
3	MG	C	403	1/1	0.95	0.07	-	22,22,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.